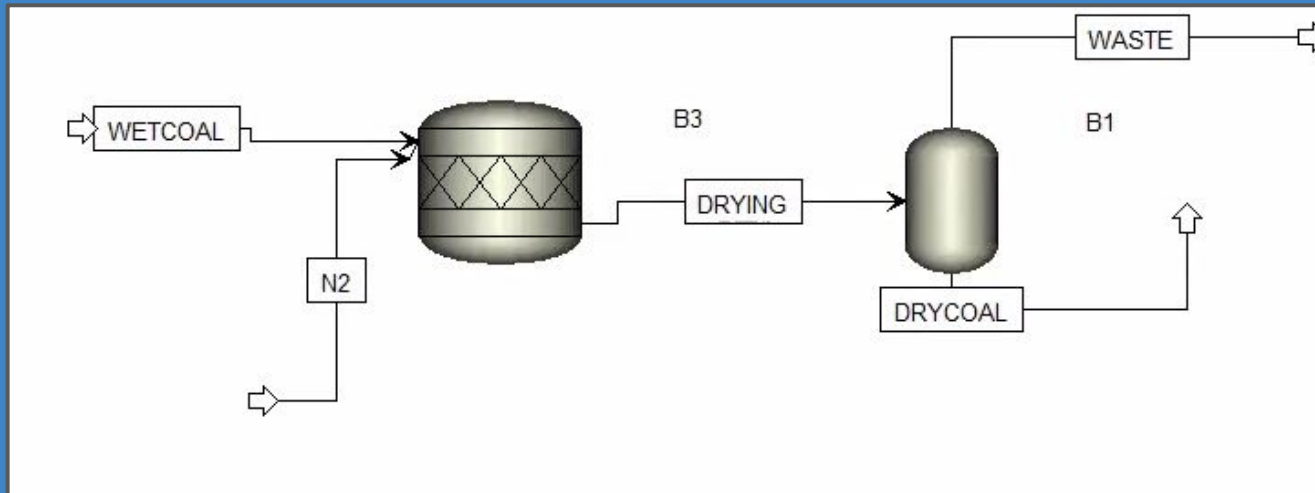


ASPEN Material Balance & Reaction of Custom Compounds

Shon, Zach, Liz, Brian, Amir, Brendon



Material Balance: The Basics

- Material balances are a prerequisite to many essential calculations when considering process design
- The laws of conservation of mass state that mass cannot be created or destroyed, but can only be transferred
- The familiar general form for a material balance is as follows...

$$\textit{Input} - \textit{Output} + \textit{Accumulation} + \textit{Generation} - \textit{Consumption} = 0$$

- Common simplifications include steady-state (accumulation = 0) and no chemical reaction (generation = consumption = 0)

Material Balance: Processes

- **Batch**
 - There is no material exchange during the process itself
- **Continuous**
 - All streams are moving in and out of the system boundaries continuously
- **Semi-Batch**
 - The process has some features of both batch and continuous processes
- **Steady-State vs. Unsteady-State**
 - In a steady-state process, process variables do not depend on time
 - In an unsteady-state process, some or all process variables change depending on when they are measured

Conventional vs. Non-Conventional Inputs

Conventional

- Pure chemical species
- Represented as molecular components
- Examples:
 - Water
 - Methane
 - Ethanol

Non-Conventional

- Solids that are not pure chemical species
- Not represented as molecular components
- Examples:
 - Coal
 - Biomass (wood, EFB, etc.)

Example Problem



Evaporation of moisture in wet coal using a hot gas stream, often containing nitrogen and oxygen

- Feed involves wet coal with 25% water content
- Goal: Dry coal with 0% water content
- Will have 2 separate water percentages
 - Initial water percentage of wet coal
 - Final water percentage of dry coal

Selecting Components for Aspen Simulation

- First step in Aspen - produce material balance
- Can change components throughout process
- Able to define your own compound

Select components

Component ID	Type	Component name	Alias	CAS number
▶ WATER	<i>Conventional</i>	WATER	H2O	7732-18-5
▶ NITROGEN	<i>Conventional</i>	NITROGEN	N2	7727-37-9
▶ OXYGEN	<i>Conventional</i>	OXYGEN	O2	7782-44-7
▶ COAL	Nonconventional			
*				

Property Methods

- Ideal, UNIFAC, Wilson
- Used to calculate thermodynamic and transport properties
- Have the ability to manually adjust as well

Methods - Specifications x +

Global Flowsheet Sections Referenced Comments

Property methods & options

Method filter: COMMON

Base method: IDEAL

Henry components: []

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID: []

Use true components

Method name: IDEAL [Methods Assistant...]

Modify

Vapor EOS: ESIG

Data set: 1

Liquid gamma: GMIDL

Data set: 1

Liquid molar enthalpy: HLMX82

Liquid molar volume: VLMX01

Heat of mixing

Poynting correction

Use liquid reference state enthalpy

Finalize Methods and Properties

- Helps characterize the unconventional solid and calculate the thermodynamic values
- Last step before running simulation
- Proxanal, Ultanal, Sulfanal: proximate, ultimate and sulfur analysis results

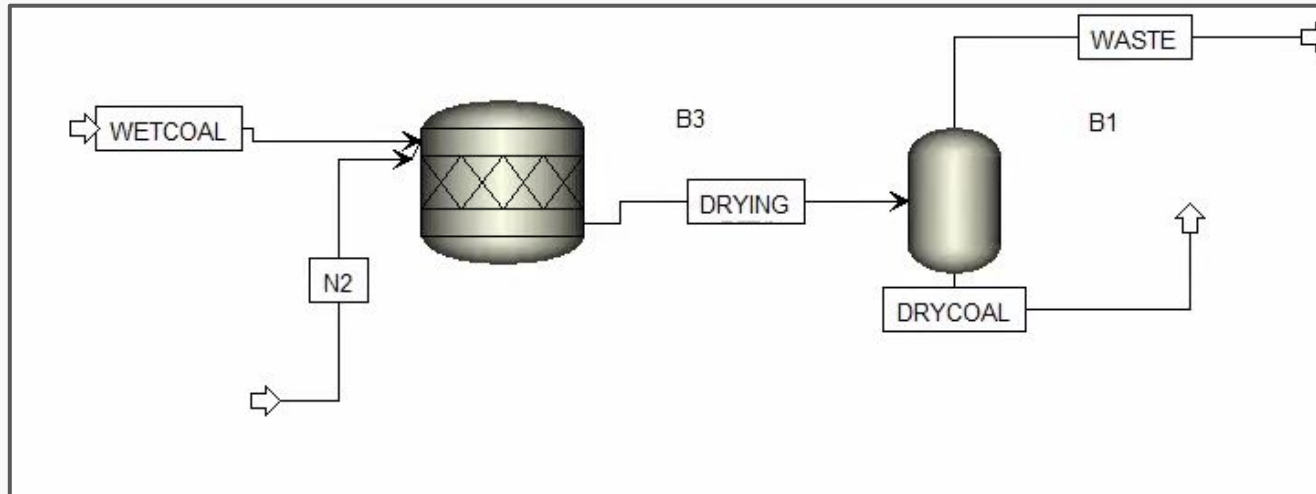
The screenshot shows the 'Methods - NC Props' window with the 'Property Methods' tab selected. The 'Component' is set to 'COAL'. Under 'Property models for nonconventional components', there is a table with columns for 'Model name' and 'Option codes'. The 'Enthalpy' row is selected, showing the model 'HCOALGEN' and four '1' option codes. The 'Density' row shows the model 'DCOALIGT' and four empty option code cells. Below this, the 'Required component attributes' section lists 'PROXANAL', 'ULTANAL', and 'SULFANAL'.

Model name	Option codes
Enthalpy	1 1 1 1
Density	

Required component attributes: PROXANAL, ULTANAL, SULFANAL

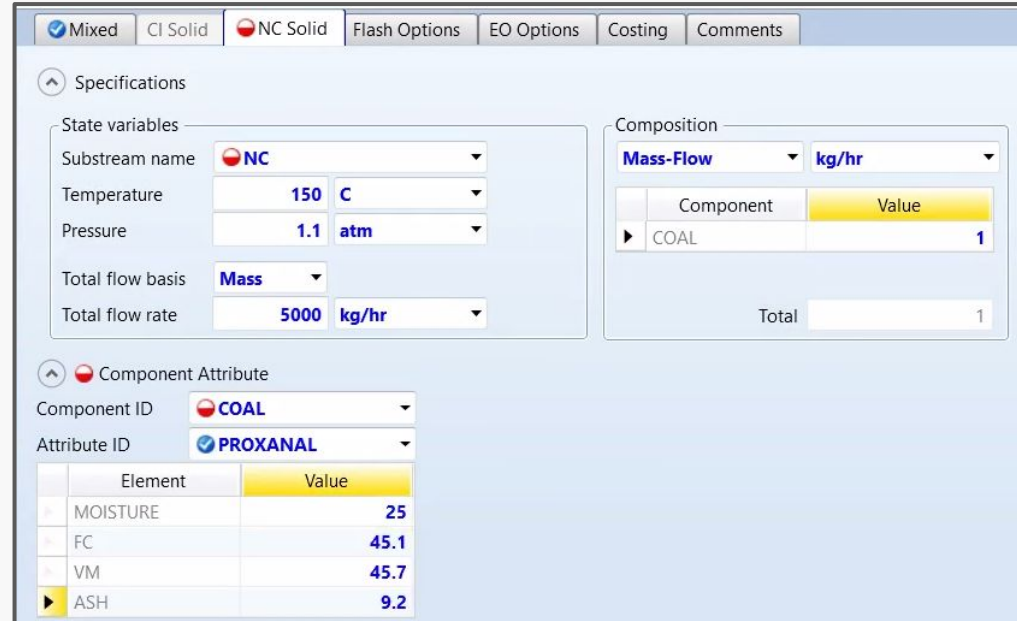
Creating the Reactor and Simulation

- Various blocks to choose from (PFR, heater, mixer, separator)
- Able to add various streams that are material, heat or water
- Add recycle stream to improve purity or recovery



Defining Feed Stream

- Various values to use
 - Will impact recovery and purity
- Have to manually input the value for each element and attribute (proxanal, ultanal, sulfanal)



Specifications

State variables

Substream name:

Temperature:

Pressure:

Total flow basis:

Total flow rate:

Composition

Mass-Flow

Component	Value
COAL	1

Total:

Component Attribute

Component ID:

Attribute ID:

Element	Value
MOISTURE	25
FC	45.1
VM	45.7
ASH	9.2

Defining First Reactor Configuration

- Temperature and pressure of reactor is flexible
- Manually enter the equation and stoich
- Purpose is to remove moisture from coal using nitrogen

Reactions						
Rxn No.	Specification type	Molar extent	Units	Fractional conversion	Fractional Conversion of Component	Stoichiometry
1	<i>Frac. conversion</i>		kmol/hr	0.2	COAL	COAL --> 0.0555084 WATER(MIXED)

Main Flowsheet x Setup x WETCOAL (MATERIAL) x N2 (MATERIAL) x **B3 (RStoic)** x +

Specifications
 Streams
 Reactions
 Combustion
 Heat of Reaction
 Selectivity
 PSD
 Component Attr.

Substream ID **NC**

Component attributes

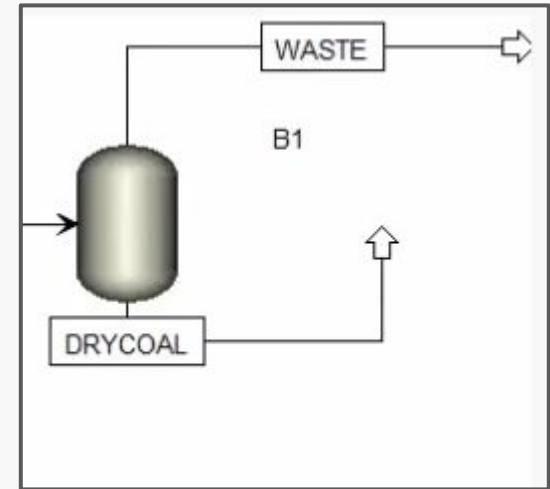
Component ID **COAL**

Attribute ID **PROXANAL**

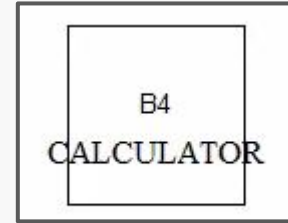
Element	Value
▶ MOISTURE	1
▶ FC	
▶ VM	
▶ ASH	

Defining Second Reactor Configuration

- Purpose of second block is to separate waste materials from dry coal
- Want a low pressure to be effective and eco-friendly



Calculator Block



- Allows you to import equations to calculate the conversion
- Have to manually put in the variables

$$\underline{\text{Conver}} = \frac{H2O_{in} - H2O_{Dry}}{100 - H2O_{Dry}}$$

The screenshot shows the configuration window for the Calculator Block. It includes a table of variables, a list of actions, and detailed settings for the selected variable.

Variable	Information flow	Definition
H2OIN		Compattr-Var Stream=WETCOAL Substream=NC Component=COAL Attribute=PROXANA...
CONVE		Block-Var Block=B3 Variable=CONV Sentence=CONV ID1=1

Buttons: New, Delete, Copy, Paste, Move Up, Move Down, View Variables

Edit selected variable

Variable: **H2ODRY**

Category:

- All
- Blocks
- Streams
- Model Utility
- Property Parameters
- Reactions

Reference:

- Type: **Block-Var**
- Block: **B3**
- Variable: **COMPATT**
- Sentence: COMP-ATTR
- ID1: **NC**
- ID2: **COAL**
- ID3: **PROXANAL**
- Element: **1**

Information flow:

- Import variable
- Export variable
- Tear variable

EO input:

- Open variable:
- Description:

Review of Steps

1. **Select/Input components** (conventional and nonconventional)
2. **Input properties and methods and verify** (Ideal, UNIFAC, or Wilson)
3. **Define feed stream, non-conventional component stream**
4. **Define 1st and 2nd reactor configurations** (setup reaction scheme)
5. **Insert a calculator block** (Allows you to find coefficients)
6. **Run simulation**

Applications

- **Reactor Design** (volume, feed rates, composition of product)
- **Separation Processes** (distillations, extractions, absorptions)
- **Recycle Streams** (minimizing waste, emissions regulations)
- **Custom Formula Compounds $\text{CH}_x\text{O}_y\text{N}_z$** (biomass, coal, cells)
- **Calculating Stoichiometric Coefficients** ($a\text{C}+b\text{H}+c\text{O}+d\text{N}$)

THANK YOU

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